

Investigations of the Nonlinear Optical Phenomena in the Series of Multiatomic Compounds by the Methods of Speeds of Balance Populations and Deactivation on Pumping in the Electronic Excited States

Alexander E. Obukhov

National Research University "Moscow Power Engineering Institute", Krasnokazarmennaya st., 14. 111250, Moscow, Russia

aobukhov@fo.gpi.ru

Received 4 June 2013; Accepted 14 June 2013; Published 13 March 2014

© 2014 Science and Engineering Publishing Company

Abstract

With the help of the measurements (the methods are the NMR ^1H and ^{13}C , infrared (IR) and the UV-absorption, Raman scattering of light, the fluorescence and the phosphorescence, the pumping of the lasers and lamps, the low-temperature of the spectroscopy in the solutions and vapor and also with application by the methods of balance speeds of populations and deactivation the energy of pumping in the electronic excited states, and the spectroscopy of properties in the range $\lambda_{\text{abs,osc}}^{\text{max}} = 208 - 760 \text{ nm}$ have been investigated. Therefore, creation of the complex methods of studying the NMR-magnetic and the optical properties at variations of the electronic and spatial structures in the series three-, penta- and quindicycles from bi- and bis- of phenyl, furyl-, thienyl- and pyridines and oxazoles and -oxadiazoles the organic compounds. The applications by the fundamental scientific problem of the formation for the quantum technologies and engineering, which allows predicting the practical synthesis of compounds with given the spatial and electronic structures and required the physical properties even before realization of practical synthesis of the luminophores.

Keywords

Spectra; Optical; Photophysic; Electronic Excited States; Dye-laser; Nanocurrent; Quantum Yields; Lifetime of Fluorescence; UV-Absorptions; NMR and IR Absorptions; Raman Scattering; Multiatomic Compounds; Dye-laser

Introductions

Wide introduction in practice of the photophysical, chemical and biological researches of various

assignment of the spectral methods of studying of the optical and magnetic properties of the organic and inorganic compounds simultaneously allows to study and widely to apply individual spectral characteristics in the vapor, solutions or crystals with the purpose of interpretation of their the nonlinear photophysical properties of the relaxation formed for time intervals from hundreds and tens up to nano-, pico-, femto- and attoseconds. Therefore, reason of the complex methods of studying of the NMR-magnetic and of the optical properties in the series multiatomic compounds for the decision of fundamental scientific problem it is formation of the new quantum model of nanotechnologies for the science and engineering, which allow to predict required properties even before realization of practical synthesis of organics luminophores. [1 - 5]

Experimental and Theoretical Methods and Materials

In article complex application of nonlinear optical phenomena in the series multiatomic compounds with the help of mechanisms the superfine electronic-nuclear interactions (SFEIN) in the singlets and triplets electronic excited states and the methods of spectroscopy were investigations. [2, 4]

Materials

All new compounds were synthesized for the decision of the given fundamental spectral problem, and their

structural formulas in papers are considered. [1 - 5]

Methods of Measurements of Spectra

The infrared absorption (IR-) spectra (λ_{abs}^{max}) in the KBr pellets is "Specord-75-IR" spectrometer, and the electronic UV-spectrums of solutions at 296 K is "Specord-M4030" spectrometers (German), and NMR ^1H and ^{13}C spectra is "Bruker"-80MGz and 250MGz were measured. Were also used X-ray structural data on the equilibrium of the nuclear configuration in the singlet ground state (S_0 , GrSt) [2, 6]. The fluorescence (Fl) spectrums (W_{fl}^v / ν^3 , λ_{osc}^{max}), and the fluorescence quantum yields, (QYFl) γ_{fl} , and lifetimes, (LtFl) τ_{fl} , is "SLM-4800S" (USA) spectrafluorimeter were measured. The duration of fluorescence (Fl), τ_{fl} , with the use of the two techniques: phase and modulation of the methods was measured. The generation radiated of light (GRI) the properties during pumping of solutions of the complex molecules in a transverse arrangement by a "Lambda Physic" excimer laser (Canada), which could provide a single pump pulse, $\Delta\tau_{exit}^{1/2}$, power density of more then, $E_{exit} \geq 0,1-35$ mJ/cm² were measured. The wavelengths of the laser pump-pulse were used: $\lambda_{exit} \approx 308$ nm (XeCl*), $\lambda_{exit} \approx 248$ nm (KrF*), $\lambda_{exit} \approx 337$ nm (gas N₂). [1 - 5]

The Spectroscopy of Ground States

The mechanisms of superfine a fermi-contact electron-nuclear interaction FC-SFEINIn arises that the nucleus has the magnetic dipole of moment of the spatial and electronics structure of multiatomic compounds in Tables 1, 2 and 3.

The Fermi-contact and Dipole-dipole of Superfine Electron-nuclear Interactions of Mechanisms in the NMR-spectra

At research of the NMR spectrums of compounds in grounds states (S_0 , GrSt) it is necessary to take into account, that contribution to the constant of shielding σ_i^{scr} (in the chemical shifts is chsh) for each nucleus ($H_0(1-\sigma_i^{scr})$) in molecule or the complex in NMR spectra as function of which is directly proportional to the square ($\Delta\rho_{\pi\sigma\ln Z}^{oi}$) to the EfTED and is inversely proportional to the cube of distances ($1/R_i^3$) between the valent of bonds by the ratio

$$\Delta\sigma_i^{screen} = -(\mu_0/4\pi) \left((\Delta\rho_{\pi\sigma\ln Z}^{oi})^2 r^2 / 2m_e R_i^3 \right). \quad (1)$$

According to statement of fundamental problem [1,2,4] for the nucleus ^1H and ^{13}C in similar positions in the spatial structure of compounds of the GrSt in the NMR spectrum average of the value SFEINIn, and always change in ranks of bonds, that is determined by character localization of the full EfTED ($\rho_{\pi z}^{oi}$) on the atoms owing to presence the ratio

$$\langle A \rangle = -(\mu_0 h / 6\pi^2) \gamma_s \gamma_I |\psi(0)|^2 = (4/3) \pi \beta q_N \alpha \beta_N (\rho_{\pi z}^{oi}) / K \int \psi^2 \sum_i [2S_{\mu\nu} \delta(N)] \psi d\psi, \quad (2)$$

where β_N is the Bore's-magneton, $S_{\mu\nu}$ is the integral by exchanges between overlaps for μ and ν nucleus, backs of nucleus is $\vec{I}$ and is $\vec{s}$ electron, $\psi(0)$ is wave functions or the EfTED on the nucleus.

The electron has the spin-magnetic moment that determines other fundamental mechanism is the spatial dipole-dipole DD-SFEINIn with the magnetic field of the own nucleus, and also others nucleus in the spatial structure of compounds representations by formula

$$F_i(\theta_i, \phi_i, r_i) = \langle D_1^{ax} \times (3\cos^2\Omega_i - 1) / r_i^3 \rangle + \langle D_2^{nax} (\sin^2\Omega_i \cos 2\alpha_i / r_i^3) \rangle, \quad (3)$$

where D_1^{ax} and D_2^{nax} is coefficients of anisotropy of the magnetic susceptibility which can be determined by the following expressions as

$$D_1^{ax} = [\beta_e S_{Ze} (S_{Ze} + 1) / 45KT] \times (3g_{II} + 4g_{\perp})(g_{II} - g_{\perp})$$

and $D_2^{nax} = -1/2(\chi_x - \chi_y)$, here g_e and g is the electron factor of Lande's, β_e is Bore's magneton, $g_{\perp}$ and g_{II} is perpendicular and parallel components of g -factor, S_z is total backs, K is the Boltzman's constant, T K is the absolute temperature, χ_x and χ_y is the magnetic susceptibility of the complex along axes oX and oY , Ω_i , α_i , r_i is spherical coordinates of the nucleus and r_i is distance between the spin-spin interactions (SpSpIn) of nucleus in spatial structure is observed.

The stereo-specific of the geminale SpSpIn between interactions of the nucleus, are defined from the following is ratio

$$^3J_{CH} = K_H K_C \times \sum_i^{HOMO} \sum_j^{LFMO} \Delta E_{ij}^{-1} (C_{i,2S} C_{j,2S} C_{i,1S} C_{j,1S})^2, \quad (4)$$

where $\Delta E_{ij} = \varepsilon_j - \varepsilon_i - K_{ij}$ is the gap energy between the highest occupied (*HOMOs*) and the lowest free the molecular orbitals (*LMOs*) in relation of GrSt S_0 , C_{ij} is the coefficients by calculations the LCAO-MO SCF expended-CI INDO/S methods.

Let's note, that for the series of phenyl-, furyl- and thienylbisoxazole (OPO, OFO, OTO, and also POPOP, FOPOF, TDPDT and others) nucleus of carbon and the protons located symmetrically concerning the vertical axis (C_{2v}) of the second order have equal of vicinale SpSpIn and geminale SpSpIn and also that defines $\sum_i \rho_{\sigma\pi, Z}^{oi}$ on the atoms in the structure (i.e. carbons, sulfur, nitrogen, and other), them as equivalent groups quasi-oscillators. [1 - 5]

Similar results for the pyridine-containing of compounds ([1-4]azafluorene) are observed. [4]

The studying of NMR-spectra in solutions has shown that the compounds, of incorporating the oxazole or oxadiazole, pyridines cycles with the central of benzene cycles in the spatial structure, have high of aromatics.

The Atomic-nano-current in the Structure

In the quantum mechanics the EfTED ($\sum_i \rho_{\sigma\pi, Z}^{oi}$) located on the atoms of the spatial structure of compounds in shares of the ones of electrons (e) that it is possible to receive the similar form of expression for size of force of the current i_{icur} for $\sigma\pi^*, \pi\pi^*$ -electron of the atoms of the carbon in the several heterocyclic is defined and thus, secondary magnetic field $B' = -B_0 \sigma^{scr}$ in the NMR spectrometer of this dipole action on the proton atoms located on distance R_i from the centre of the cycle is equal $\mu = R_i^3$ and can be determined from expression

$$B' = -(\mu_0/4\pi) B_0 \left(3 \left(\Delta \rho_{\pi\sigma \ln Z}^{oi} \right)^2 r^2 / 2m_e R_i^3 \right) \quad (5)$$

where σ^{scr} is the constant of shielding of the each nucleus in the structure of compounds.

For the investigated compounds in the GrSt (S_0) the values EfTED on different types of the atoms is the source (the nano-quasioscillators of minimal size) weak by the electric nanocurrent. [2,4]

Thus, in the atomic models for the multinuclear compounds transfer of the logic-spectral information can be carried out only by change of the nature of mechanisms SFEINIn from the donor to the acceptor

which the formed by of a spatial and electronic structure.

Raman Scattering and Infrared Absorptions Spectra

According to the carried out researches in the IR-absorption and Raman scattering in the series poly- and heteroaromatic compounds in the singlet GrSt in the range of the frequencies is (3600 - 3100 cm^{-1} and 1600 - 1630) cm^{-1} and (1540 - 1534) cm^{-1} should correspond to the most high-frequency and intensive combinational strips by the symmetric and the nonsymmetric types is double and unary $\leq C-H$, $=N-N=$, $=C-C=$, $=C-N=$, $>C=C<$ is 415, 495, 530, 695, 720, 772, 810, 858, 910, 980, 1015, 1075, 1110, 1180, 1255, 1305, 1320, 1350, 1420, 1440, 1490, 1530, 1562, 1580, 1620, 2800-3200 cm^{-1} and the intensive of vibration-deformations or nonfullsymmetry and fullsymmetry of valent bonds in oxazoles and oxadiazoles cycles is B_{1U} , B_{2U} B_{3U} types arises are observed. [2,4,7]

The more rotary and oscillatory degrees of freedom typically for a given of spatial configuration, and thus, there the instability of spatial structure in vapor and solutions is more.

The Spectroscopy of Electronic Excited States

In the quantum theory mechanisms of nonlinear optics and spectroscopy can be considered with application the UV-quantum model of speeds of balance populations which allows from establish of the photophysical properties in different conditions are investigations in Fig. 1.

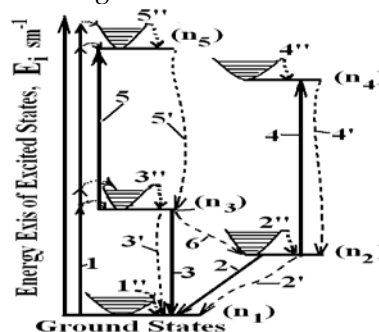


FIG. 1. THE FIVE-LEVELS SYSTEM FROM THE MULTI-ATOMIC MOLECULES. (1) IS THE PROCESS ENERGY OF LASERS PUMPING, (2 AND 2') IS PHOSPHORESCENCE OF THE RADIATION AND NONRADIATED TRANSITIONS, (3 AND 3') IS OF THE FLUORESCENCE OF RADIATION AND THE NONRADIATED TRANSITIONS, (4 AND 5) THE SINGLET-SINGLET AND THE TRIPLET-TRIPLET REABSORPTION OF TRANSITIONS, (2', 3', 4' AND 5') THE INNER COMBINATION CONVERSIONS OF TRANSITIONS, (1'', 2'', 3'', 4'', 5'') OR (PICoseconds OF THE ELECTRON-VIBRATION RELAXATION), (6) IS INTERCOMBINATION CONVERSIONS OF TRANSITIONS.

The Models Speeds of Balance of Populations

When organic molecules are excited with UV pumping sources with a radiation energy $> 3 - 4$ eV and the lines corresponding to $S_3^* \rightarrow S_5^*$ and $T_2 \rightarrow T_4$ electronic transitions arise in the spectra of singlets and triplets electronic excited states before photon emission, these transitions play a dominant role in the formation of the gain strips, the lasing, and the multistage processes of multistrips photoionization in Fig. 1. [1, 2, 9, 10]

For a quantum particle with the three- and five-levels scheme if vibration parameters of the connected dye [(compounds+solutions)+ resonator] satisfy in dye-laser to a ratio

$$\chi_{31}(\nu^{osc}) = \frac{[K_{ampl}(\nu^{osc}) - \chi_{35}(\nu^{osc}) - \chi_{24}(\nu^{osc})] \frac{p_{32}}{p_{31}}}{p_{31}} \quad (6)$$

where is $K_{ampl}(\nu)$ initial coefficient of losses of the resonator, $\chi_{31}(\nu^{osc})$, $\chi_{35}(\nu^{osc})$ and $\chi_{24}(\nu^{osc})$ limiting coefficient of amplification and the singlet-singlets and triplet-triplets reabsorption spectra in dye-laser. [2]

Here the ratio $p_{31} = 1/k_{\beta} = 1/k_{31} \approx \tau_{\beta}/\gamma_{\beta}$, and, $p_{32} = 1/k_{32} \approx \tau_{\beta}/(1-\gamma_{\beta})$ are the probabilities of the radiation and non-radiation transition and less decay of the FI-spectra (State S_1^*) and Ph-spectra (State T_1) levels: $\tau_{\beta} = 1/\tau_{\beta}^0$, and $\tau_{ph} = \gamma_{ph}/\gamma_T \tau_{ph}^0$, where τ_{β} , γ_{β} , and γ_T is measurement the radiating lifetime (RLtFI)

and quantum yield FI (QYFI). [1]

The cross sections of the transitions between the interacting of the five levels in dye-laser (or OLEDs) at the wavelengths of pumping and lasing $\sigma_{2TT,3SS}^*(\nu^{exit,osc})$ are used as parameters in the latter formula as

$$K_{ampl}(t, \nu) \equiv \sigma_{31}^{osc}(\nu) n_3(t) \geq \sigma_{13}^{abs}(\nu) n_1(t) + \sigma_{24}^{reabs}(\nu) n_2(t) + \sigma_{35}^{reabs}(\nu) n_3(t) + K_p^0(t, \nu) + \rho'(\nu) \quad (7)$$

where $\sigma_{31}^{osc}(\nu)$ is the stimulated emission cross section (or the GRI) and $\sigma_{13}^{abs}(\nu)$, and $\sigma_{24}^{reabs}(\nu)$, $\sigma_{35}^{reabs}(\nu)$ are the cross sections of UV-absorptions and $S_1^* \rightarrow S_5^*$, and $T_1 \rightarrow T_4$ -reabsorption spectra and on laser excitation frequency $\nu^{osc,exit}$ at the electronic multistage transitions are $S_0 \rightarrow S_1^* \Leftrightarrow S_1^*$, $S_1^* \approx T_1$, $S_1^* \rightarrow S_5^*$, $S_1^* \Leftrightarrow S_5^*$, $T_1 \rightarrow T_4$ and $T_1 \Leftrightarrow T_4$, $T_1 \Leftrightarrow S_1^*$ in the full spectra of STElExSt.

Thus, one should know the form of the spectral functions $\sigma_{31}^{osc}(\nu)$, $\sigma_{13}^{abs}(\nu^{exit})$, $K_{ampl}(\nu^{osc})$, $\sigma_{35}^{reabs}(\nu^{osc,exit})$, $\sigma_{24}^{reabs}(\nu^{osc,exit})$, and $\chi_{31}(\nu^{osc})$ to determine the generation radiated of lithg (GRI) and laser excitation frequency $\nu^{osc,exit}$ and the approximate threshold values of the laser limit power P_{exit} , and laser energy of limit pump-pulse E_{lp} .

The cross section of the emission also low also make $\sigma_{31}^{osc}(\nu) \approx 10^{-19} - 10^{-18}$, cm² in Table 4.

TABLE 1. THE CHEMICAL SHIFTS OF THE PHOTONS IN THE SERIES COMPOUNDS IN THE NMR SPECTRA

Compounds	Chemical shifts of protons, chsh (ppm)				
	Number of atoms				
	H ₍₄₎ (a)	H ₍₅₎	H _(3')	H _(4')	H _(5')
2-(2-phenyl)-oxazol-5-formilcarboaldehyd (PO-COOH)* (signal -COH)	7,07s (9,75s)*	-	6,87dd	6,35dd	7,45d.wid.
2-(2-thienyl)-oxazol-5-carboaldehyd (FO-5-COH)*	8,07s (9,8s)*	7,51s	6,79dd	7,94dd	7,85m
2'-phenyl-2,5'-bioxazol (POO)	7,17s				-
2'-(furyl-2)-2,5'-bioxazol (FOO)	7,39d	8,37d	7,27 dd	6,74dd	7,40m (3H)
2'-(thienyl-2)-2,5'-bioxazol (TOO)	7,41s	8,12s	7,85 dd	7,27dd	7,88dd
1,4-phenylen-2,2'-bisoxazol (OPO)	7,76s	8,12s	7,3s (4H)	-	7,79dd
1,4-furylene-2,2'-bisoxazol (FOFO)	7,36s	8,08s	7,25s (2H)	-	7,4 m (3H)
1,4-thienylen-2,2'-bisoxazol (OTO)	7,6s	7,92s	7,23s (2H)	-	7,4 m (3H)

The note: The signals of protons look like overlapped multiplets $J_{45} = 7 \div 8$ Gz, (*) in solution CCl₄ and (**) in the solution CDCl₃. In the spectrum on frequency 250 MGz splitting protons of oxazole cycle $J_{45} = 0,7$ Gz, and also in thiofene cycle $J_{34} = 3,5$ Gz is observed; $J_{35} = 1,0$ Gz; $J_{45} = 5$ Gz and in thiofene cycle $J_{34} = 4$ Gz, $J_{35} = 1,5$ Gz, $J_{45} = 5,5$ Gz, (e) in furane cycle $J_{35} = 3,5$ Gz, $J_{34} = 2,5$ Gz, (j) is CSSI J_{45} and J_{35} but in spectrum NMR ¹H on frequency 60 and 80 MGz are not shown.

TABLE 2. THE CHEMICAL SHIFTS OF THE PHOTONS IN THE SERIES [1-4]-AZAFLUORENES IN THE NMR SPECTRA

Compounds	Solutions	Numeration of protons, J(Gz)									
		H ₍₁₎	H ₍₂₎	H ₍₃₎	H ₍₄₎	H ₍₅₎	H ₍₆₎	H ₍₇₎	H ₍₈₎	9-CH ₂	3-CH ₃
[1]-azafluorene	acetone-d ₆	-	8,25	7,11	7,93	7,67	7,2	7,17	7,42	3,85	
	CDCl ₃	-	8,29	7,08	7,77	7,58	7,2	7,18	7,37	3,88	
	DMSO	-	8,32	7,18	8,07	7,6	7,25	7,28	7,45	3,94	
[2]-azafluorene	acetone d ₆	8,7	-	8,48	7,70	7,81	7,31	7,37	7,58	4,1	-
3-Metyl-[3]azafluorene	Acetone-d ₆	8,6			7,41	7,7	7,2	7,21	7,39	3,94	2,61
	CDCl ₃	8,43	-	-	7,03	7,58	7,17	7,17	7,37	3,75	2,55
	DMSO	8,50			7,6	7,68	7,16	7,17	,36	3,88	2,58
[4]azafluorene	Acetone-d ₆	7,74	7,09	8,38		7,89	7,31	7,28	7,46	3,58	
	CDCl ₃	7,64	7,04	8,47		8,01	7,34	7,3	7,44	3,71	
	DMSO *	7,86	7,2	8,42		7,88	7,35	7,33	7,54	3,88	

TABLE 3. THE CONSTANT OF THE SPIN-SPIN INTERACTIONS (CSPSPIN) BETWEEN THE PROTONS IN THE SERIES [1-4]-AZAFLUORENES IN THE NMR SPECTRA IN SOLUTIONS CDCL₃

Compounds	Numeration interactions of protons, J(Gz)								
	J ₍₂₋₃₎	J ₍₂₋₄₎	J ₍₃₋₄₎	J ₍₅₋₆₎	J ₍₅₋₇₎	J ₍₅₋₈₎	J ₍₆₋₇₎	J ₍₆₋₈₎	J ₍₇₋₈₎
[1]-azafluorene	4,9	1,6	7,5	7,6	1,0	0,8	7,6	1,1	7,5
[2]-azafluorene	-	-	7,1	7,7	1,2	0,7	7,5	1,1	7,6
[4]azafluorene	4,8	J ₍₁₋₃₎ 1,5	J ₍₁₋₂₎ 7,5	7,4	1,3	0,8	7,1	1,0	7,4

Thus, the QYFI γ_{fl} and LtFI τ_{fl} , which can be measured experimentally for given conditions, contain the information concerning the net effect of external factors on an compounds, although all the formulas involve parameters of innermolecule processes (the rate constants k_{nr}) related to one quantum of absorbed and one quant of emitted the fluorescence and phosphorescence in Table 1.

Variations of the Spectral-luminescence and Generation Radiated of Light Propertie

In these chapters of connection among themselves the spectral, luminescent and the GRI properties of the multinuclear compounds which can be applied in UV-dye-lasers (OLEDs) or as the biological molecules will be considered. [11]

This analysis will be based the spectral-fluorescence characteristics at the variations in the series of electron and spatial structure compounds in vapors and, solutions were measured in Table 4.

Variations the Series of Tri- and Pentacycles of Compounds

The shortest lasing wavelength were found in **2-PO-5-COOH** and **2-PO-5-COOCH₃** (compounds 1 and 2), $\lambda_{gen}^{max} = 335$ nm, and, $\lambda_{gen}^{max} = 344$ nm in DiEG at high threshold the limit energy of density dye-laser, $E_{lp} = 8.0$ mJ/cm², respectively in Fig. 2.

Of the complex molecules is the paraterphenyl (**PPP**), and 2,5-diphenyl-1,3-oxazole (**POP**) the GRI efficiently

in solution is compounds 3 and 4 in Fig. 3.

The molecules 2,5-diphenyl-1,3,4-oxadiazole (**PDP**) in ethanol solutions and for density vapor 2,5-diphenylfuran (**PFP**) QYFI $\gamma_{fl} = 0.84$ and 0.62 and at threshold energy of density $E_{lp} = 0.2 - 0.35$ mJ/cm², respectively.

The value thresholds of the laser pump-pulse E_{lp} , falls in the transition from the bi- to corresponding the phenyl-, furyl-, thienyl- tricycles bis-oxazoles by the molecules is **POO**, **FOO**, **TOO** of compounds 5, 6, 7, to **OPO**, **OFO**, **OTO** is compounds 8, 9, and 10.

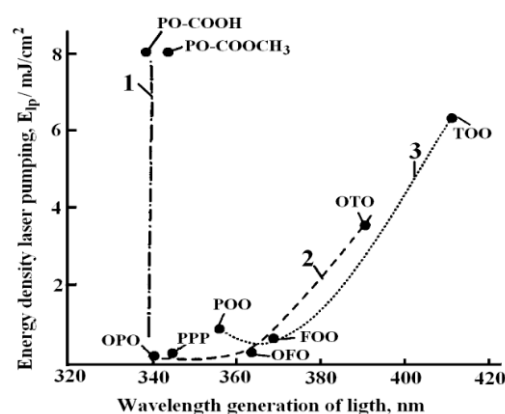


FIG. 2. THE DEPENDENCE OF THRESHOLD PUMP ENERGY DENSITY E_{lp} ON THE LASING WAVELENGTH 320 - 420 NM IN SOLUTIONS OF ETHANOL FOR THE COMPOUNDS (STOKE - DASHED LINE 1) ARE **PO-COOH**, AND **PO-COOCH₃** (CONTINUOUS LINE 1); THE SERIES PHENYL-, FURYL-, THIENYL BISOXAZOLES ARE **OPO**, **OFO**, **OTO** (CONTINUOUS LINE 2) AND SERIES THE PHENYL-, FURYL-, THIENYL BIOXAZOLES ARE **POO**, **FOO**, **TOO** (CONTINUOUS LINE 2) FOR THE "CRITICS OF RANGE" ARE 320 - 340 NM IN THE UV-SPECTRA.

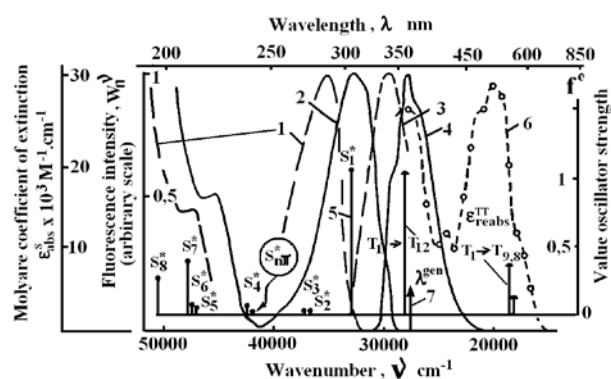


FIG. 3. THE ABSORPTIONS (ϵ_{abs}^1 , 1, 2) (1) IS VAPOUR AND (2) SOLUTIONS IN ETHANOL FOR THE MOLECULE 2-PHENYL-1,3-OXAZOL (*POP*). (1, 2) IS LINES OF VERTICAL CONTINUOUS A SHOW FREQUENCIES AND VALUE OF OSCILLATORS STRENGTH FOR ELECTRONIC TRANSITIONS $S_0 \rightarrow S_{1,2,...,8}^*$ ($\pi\pi^*$, $\sigma\pi^*$, $n\pi^*$ -TYPES) IN THE UV-ABSORPTIONS SPECTRA, (5) IS 0-0-TRANSITIONS, (3, 4) IS THE $T_1 \rightarrow T_{1,...,12}$ TRANSITIONS OF THE INDUCED OF LASER REABSORPTIONS OF SPECTRA BY CALCULATIONS THE LCAO-MO SCF EXTENDED-CI INDO/S METHODS [1].

The series of tricycles molecules in solvent ethanole+H₂SO₄ of FI-spectra within the visible spectral region in the wavelength range to $\lambda_{gen}^{max} = 390 - 420$ nm and with QYFI $\gamma_{fi} = 0.54 - 0.61$, but do not GRI even at the high density pump-pulse E_{lp} of laser in Fig. 2.

For example, for the series of bisoxazole is **OFO** (compounds is 9) and bioxazoles is **FOO** (compounds is 6) with different QYFI $\gamma_{fl} = 0.63$ and $\gamma_{fl} = 0.36$ in ethanol of solutions, respectively, and also GRI and different thresholds a laser-pump-pulse $E_{lp} = 0.33$ and 0.73 mJ/cm^2 , respectively in Fig. 2.

At excitation of solution of the 1,4-phenylene-2,2'-bisoxazole (*OPO*) (compounds is 8) by the laser pulse duration of 10 ns and wavelength of $\lambda_{exit}^{max}(\nu) = 308$ and 248 nm, the new dye-laser with minimally possible size of a threshold energy of pump density $E_{lp} \approx 0,1 - 0,5$ mJ/cm² is received [1].

The latter is lower than the *PPP*-molecule the GRI with parameters is $\lambda_{gen}^{\max} = 340$ nm and, $E_{lp} = 0.25$ mJ/cm² in the ethanol, and thus, it is higher, than the value E_{lp} for the *OPO* $E_{lp} = 0.14$ mJ/cm² under of the same experiments in Fig. 3.

density pump-pulse of laser. [1,2]

When for the *OPO* used as the solvent of 1,1,2,2'-trifluoroethanol we have, to parameter for dye-lasers are $E_{fp} < 0.1 \text{ mJ/cm}^2$, and, $\lambda_{gen}^{\max} = 340 \text{ nm}$.

This is the only example known so far of simultaneous shortening the wavelength of GRI and lowering the value E_{lp} for the UV-dye-laser.

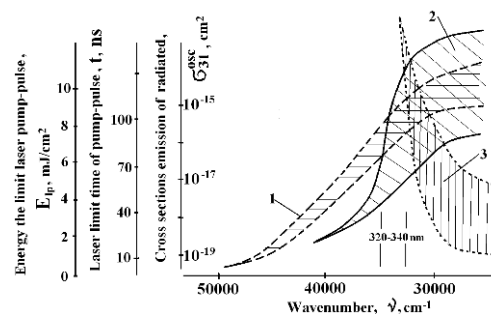


FIG. 4. THE NONLINEAR DEPENDENCE: THE LINE 1 - $\sigma_{31}^{osc}(\nu^{\max})$ ARE THE CROSS SECTIONS THE RADIATED OF LIGHT, LINE 2 - t_{lp} IS THE LIMIT TIME OF FIRST FRONT DURATIONS OF LASER PUMP-PULSE, LINE 3 - E_{lp} IS THE LIMIT THRESHOLD ENERGY OF DENSITY OF LASER PUMP-PULSE FOR "CRITICS OF RANGE" IN THE 320 - 340 NM AND OF RANGE 200 - 760 NM IN THE UV- AND VISIBLE SPECTRUM ARE MEASURED.

The series of pentacycles N-,O-,S-heteroaromatic compounds is 1 - 24 of FI-spectra within the visible spectral region in the range $\lambda_{gen}^{max} = 388 - 560$ nm with QYFI $\gamma_{FI} = 0.33 - 1.0$ in Table 4 [1, 2].

When *-OPO-*, *-OFO-*, *-DPO-*, and *-DPD-* (compounds 25 - 34) are employed as central fragments in the pentacycles of compounds that the QYFI may range from $\gamma_{FI} = 0.6$ to 1.0 depending on the properties of solvents.

If *-OTO-*, *-DTO-*, and *-DTD-*, or other laser-active compounds are employed as central fragments in compounds 32, 33, 34 (is *POTOP*, *POTDP*, *POTDT*), i.e., when the thiophene of cycles in centre of the spatial structure, then we have QYFI $\gamma_{fl} = 0.36$ to 0.47 depending on the properties of solvents is positioned, and these compounds GRI with $P_n = 4.22 - 5.3$ mJ/cm².

The pentacycles of compounds in solvent ethanole+H₂SO₄ (of complexis and protonated) of FI-spectra within the visible spectral region in the wavelength range $\lambda_{gen}^{max} = 480 - 528 - 760$ nm with QYFI $\gamma_{fl} = 0.43 - 0.67$, but do not GRI even at high density

P_{lp} capacity pump of laser.

But, in solvent of ethanole+H₂SO₄ the Fl-intensive within the visible spectral region in the wavelength range to $\lambda_{gen}^{max} = 522 - 760$ nm with QYFI $\gamma_{fl} = 0.72 - 0.8$, but do not GRI even at high density laser.

Time of Limit of First front the Pumping Pump Laser Pulse

The simplified relationship obtained on the basis of kinetic equations of the population balance from to ratio [1]

$$t_{lp} \leq \frac{2}{k_{ST}} \frac{\sigma_{31}^{osc}(\nu)}{\left[\frac{2\tau_{fl}}{(1-\gamma_{fl})} \right] \frac{\sigma_{3SS}^{reabs}(\nu^{osc})}{\sigma_{2TT}^{reabs}(\nu^{osc})}} \approx \quad , \quad (8)$$

where k_{ST} is the RC ItCC, $\sigma_{31}^{osc}(\nu)$ and $\sigma_{2TT}^{*}(\nu^{osc})$ is the cross sections of stimulated emissions spectra and the triplet-triplets of reabsorptions spectra, respectively in the wavelength of Fl-spectra, ν_{fl}^{max} , and

τ_{fl} and γ_{fl} is the LtFl and QYFI. [1-5,10]

The **POP**-compounds in vapour the QYFI γ_{fl} decrease to $\gamma_{fl} = 0.24$ and increase QYFI $\gamma_{fl} = 0.71$ in ethanol. [1]

TABLE 4. THE SPECTRAL-FLUORESCENCE AND RADIATED OF LIGHT PARAMETERS FOR THE COMPOUNDS № 1 – 34 IN SOLUTIONS AND VAPOR ARE MEASURED, AND ALSO THE QUANTUM CHEMICAL OF CALCULATIONS BY LCAO-CSF CI INDO/S METHODS

No	Compound (abbreviation)	State of aggregation	λ_{abs}^{max} , nm	λ_{osc}^{max} , nm	γ_{fl}	ε_{abs}^{max} , 10^3 , $M^{-1} \cdot cm^{-1}$	k_{fl}^x , 10^9 , s^{-1}	k_{st}^x , 10^9 , s^{-1}	$\sigma_{31}^{osc} x$, 10^{-16} , cm^2	$\sigma_{31}^{osc} x$, 10^{-16} , cm^2	t_{lp}^x , 10^{-9} , s	$E_{lp} (P_{lp})$, mJ / (mW / cm^2)
1	2-phenyl oxazol-5-carboxylic Acid (PO-5-COOH)	ethanole	276	(326,	0,03	34,1	10^{-3}	0,10	1,31	2,5	10^{-3}	-
		DiEG	282	335)	0,18	31,5	0,08	0,36	1,41	2,87	5,9	8,0
		vapor, INDO/S	271	-	0,01	-	0,06	0,44	-	2,5	10^{-3}	-
2	methyl-ether of 2-phenyl-oxazole-5-charboxylic acid (PO-5-COOCH3)	ethanole	277	335	0,04	31,1	0,04	0,74	1,2	4,36	0,12	-
		DiEG	282	344	0,22	32,6	0,08	0,7	1,26	4,87	6,2	8,0
		vapor, INDO/S	-	-	-	0,1	0,07	0,44	-	4,0	0,007	-
3	parater-phenyl (PPP)	ethanole	276	340	0,83	30,64	0,68	0,14	1,2	2,8	96,4	0,25
		vapor, laser	258	343	0,1	30	0,10	0,90	0,23	2,6	5,7	$\geq 1,8$
		vapor, lamp	258	343	0,01	30	0,1	0,6	0,023	2,6	0,3	-
		vapor, INDO/S	258	343	0,38	30	0,1	0,87	0,1	2,6	2,8	-
4	2-phenyl-1,3-oxazole (POP)	cyclohexane	302	356	0,81	34,0	0,58	0,14	13,0	0,84	7,5	7,5
		ethanole	303	362	0,71	29,6	0,44	0,18	11,4	0,86	1,1	6,5
		ethanole+H ₂ SO ₄	314	406	0,51	21,0	0,23	0,21	0,81	0,03	0,07	0,05
		toluene	306	382	0,51	29,1	0,72	0,96	11,2	0,48	-	4,7
		vapor, lamp	289	352	0,24	9,2	0,26	0,85	0,36	0,21	1,2	1,2
		vapor, laser	290	350	0,012	9,2	0,010	1,10	0,35	0,02	0,06	0,06
		vapor, INDO/S	290	349	0,24	-	0,61	0,69	0,40	0,34	2,0	0,05
5	2-phenyl-2,5-bioxazole (POO)	cyclohexane	302	356	0,37	23,2	0,29	0,49	9,0	0,69	21,9	-
		ethanole	302	376	0,48	29,5	0,30	0,33	11,4	0,65	30,8	0,9
		ethanole+H ₂ SO ₄	317	388	0,54	24,4	0,23	0,20	9,4	0,27	0,3	-
		vapor, INDO/S	315	375	0,25	25,0	0,24	0,72	0,96	0,20	2,2	-
6	2-(furyl-2)-2,5-bioxazole (FOO)	ethanole	314	367	0,36	28,4	0,3	0,53	10,9	0,66	10	0,73
		vapor, INDO/S	296	-	0,18	-	0,54	0,96	-	0,73	0,6	-
7	2-(thienyl-2)-2,5-bioxazole (TOO)	ethanole	320	-	0,17	-32,0	0,19	0,92	1,23	0,46	1,3	-
		toluene	320	410	0,17	27,9	0,4	0,78	1,08	0,76	5,0	6,4
		vapor, INDO/S	308	-	0,08	-	0,58	2,82	1,0	0,35	0,1	-
8	1,4-phenyl ene-2,2'-bis oxazole (OPO)	1,2,2'-TFTCE*	306	340	0,93	42,2	0,93	0,07	1,63	2,08	644	$\leq 0,1$
		cyclohexane	308	344	0,60	34,6	0,60	0,40	1,33	1,38	83	0,38
		toluene	311	352	0,49	37,7	0,49	0,51	1,46	1,18	36	-
		THF	311	350	0,61	35,9	0,76	0,49	1,38	1,81	50	-
		ethanole	309	350	0,71	42,8	0,65	0,27	1,65	1,51	95	0,14
		DMFA	312	354	0,81	35,4	0,73	0,17	1,36	1,80	93	-
		DMSA	325	368	0,45	38,2	0,41	0,50	1,47	1,08	15	0,53
		DiEG	313	356	0,85	34,8	0,86	0,16	1,34	2,09	18	-
		ethanole+H ₂ SO ₄	310	420	0,61	38,2	0,28	0,18	1,47	0,83	0,2	-
		vapor, INDO/S	311	345	0,71	40	0,69	0,28	1,06	1,06	32	$\geq 0,3$
9	2,5-furylene-2,2'-bis oxazole (OFO)	ethanole	321	363	0,63	27,8	0,51	0,30	1,09	1,0	41,7	0,33
		vapor, INDO/S	303	-	0,35	-	0,26	0,15	-	0,56	3,4	-

10	2,5-thienyl ene-2,2'-bis oxazole (OTO)	toluene ethanole DMFA ethanole+H2SO4 vapor, INDO/S	341 338 339 346 336	395 390 392 418 -	0,14 0,21 0,14 0,42 0,01	0,25 0,35 0,26 0,19 0,02	0,78 1,32 0,79 0,26 18,5	1,32 0,78 0,79 0,26 0,26	1,1 0,97 0,84 0,97 0,99	1,05 0,41 0,40 0,03 0,51	0,43 0,40 0,41 0,01 0,09	0,4 0,43 0,41 0,1 0,01
11	5-(para-aminophenyl)- 2-phenyl-1,3-oxazole (5- <i>p-NH₂-POP-1,3</i>)	toluene	329	388	0,58	32,4	0,48	0,35	1,25	0,34	10,3	-
12	2-(para-aminophenyl)- 2-phenyl-1,3-oxazole (2- <i>p-NH₂-POP-1,3</i>)	toluene	328	389	0,54	33,1	0,45	0,39	1,28	0,4	10,4	-
13	2-(orto-amino phenyl)- 2-phenyl-1,3,4- oxadizole (2- <i>o-NH₂- PDP-1,3,4</i>)	ethanole toluene	357 351	435 404	0,63 0,59	27,9 29,1	0,30 0,35	0,18 0,17	1,08 1,12	0,23 0,20	3,35 7,42	- -
14	2-(para-aminophenyl)- 2-phenyl-1,3,4-oxa Dizole (2- <i>p-NH₂-PDP- 1,3,4</i>)	vapor, lamp toluene	304 349	355 380	0,24 0,68	25 27,5	0,34 0,55	0,40 0,26	0,96 1,06	0,4 2,9	3,1 23,3	- -
15	2-(para-dimetyl aminophenyl)-2- phenyl-1,3,4-oxadia zol (2- <i>p-di-(CH₃)₂-PDP- 1,3,4</i>)	ethanole DMFA	334 336	364 368	0,52 0,56	28,1 29,4	0,52 0,56	0,01 0,07	1,08 1,13	1,22 1,63	43,1 39,5	- -
16	2-di-(para-metoxi- phenyl)-2-phenyl-1,3,4- oxadizole (2- <i>di-p- OCH₃-POP-1,3,4</i>)	ethanole laser, vapor	303 283	363 343	0,57 0,20	26,5 25,0	0,38 0,11	0,63 0,44	1,02 0,96	2,63 0,56	23,7 28,6	- -
17	2-di-(para- aminophenyl) phenyl- 1,3,4-oxadiazol (2- <i>di-p- NH₂-PDP-1,3,4</i>)	toluene ethanole DMFA	353 340 342	376 403 402	0,58 0,80 0,67	27,4 31,2 32,4	0,55 0,53 0,48	0,40 0,13 0,24	1,06 1,20 1,25	3,94 2,4 2,94	59,3 52,0 41,9	- - -
18	2-di-(para- metoxi- phenyl) phenyl-1,3,4- oxadiazol (2- <i>di-p- OCH₃-PDP-1,3,4</i>)	laser, vapor ethanole ethanole+H2SO4	281 316 370	330 357 426	0,17 0,57 0,23	25 28,4 24,2	0,08 0,38 0,10	0,40 0,29 0,34	0,96 1,10 0,94	0,52 2,55 0,51	1,9 32,4 5,7	- - -
19	2-di-(orto-oxiphenyl) phenyl-1,3,4-oxadiazol (2- <i>di-o-OH-PDP-1,3,4</i>)	ethanole ethanole+KOH	341 364	397 449	0,49 0,15	27,7 24,3	0,27 0,07	0,28 0,38	1,07 0,94	1,2 0,11	3,5 0,13	- -
20	2-di-(orto-amino phenyl) phenyl-1,3,4- oxadiazol (2- <i>di-o-NH₂- PDP-1,3,4-</i>)	ethanole	369	406	0,51	25,6	0,34	0,33	0,99	0,37	3,97	-
21	2-phenyl-1,3- benzoxazole (2 <i>PbO</i>)	laser, vapor cyclohexane	298 300	312 328	0,24 0,78	25 26,9	0,1 0,43	0,90 0,12	0,96 1,04	0,04 0,14	0,07 9,73	- -
22	2-(orto-aminophenyl)- 1,3-benz oxazole (2- <i>o- NH₂-PbO</i>)	toluene	324	348	0,58	27,1	0,36	0,26	1,04	0,22	5,31	-
23	paraquater-phenyle (PPPP)	ethanole	298	367	37,9	1,46	0,91	0,83	0,008	3,22	87,4	0,51
24	2,5-phenyl-5-(4-bi phenyl)-1,3,4-oxa diazole (PDPP)	ethanole	305	376	39	0,88	0,88	0,12	1,5	2,88	68,4	1,87
25	2,5-di-biphenyl-1,3,4- oxa diazole (PPOPP)	ethanole	340	409	51,2	0,89	0,75	0,92	1,97	2,24	73,1	0,45
26	2(phenylbenz-1,3- oxazolyle-2)benzole (BboPobB)	laser, vapor highlydense vapor, laser chloroforms toluene	318 337 341 373	- 393 (377; 397; 417) (373; 393,5; 446,5)	0,65 0,6 0,9 0,9	53,3 50,0 53,3 50	0,54 0,66 0,64 0,64	0,29 0,45 0,07 0,07	2,1 1,5 2,1 1,9	1,63 1,46 2,19 1,46	37,5 97,5 98,1 91,7	0,25 (0.1- 0.58) 0,8 0,9

27	1,4-di-(5-phenyl oxazolyl-2) benzole (POPOP)	toluene	366	418	0,86	52,3	0,72	0,12	20,1	3,72	68,7	(2,34)
		ethanole	360	422	0,97	54,5	0,60	0,04	21,0	2,26	96,4	(2,2)
		ethanole+H2SO4	373	508	0,93	39,3	0,43	0,09	15,0	1,39	0,1	-
		Highlydense vapor	324	383	0,80	70,0	0,86	0,22	26,8	2,83	43,0	
		vapor, laser(266 nm)	324	392	0,06	66,8	0,07	1,04	27,0	0,53	4,0	
		INDO/S	319	379	0,80	-	0,96	0,22	27,8	2,79	39,2	
28	2-[(5-phenyl oxazolyl-2)-5-(5-phenylyl - 2)]benzole (POPDP)	toluene	351	412	51,9	0,93	0,69	0,05	2,0	1,94	68,9	2,25
		ethanole	318	378	53	0,8	0,89	0,22	2,04	2,17	55,1	2,63
29	1,5-phenyl oxazolyl-2-4-[5-(furyl-2)-1,3,4-oxa diazoly-2] benzole (POPDP)	ethanole	351	440	46,7	0,9	0,69	0,08	1,8	2,61	36,3	2,3
		toluene	352	434	44,2	0,91	0,7	0,07	1,9	2,48	49,6	2,2
		dioxane	352	414	50,8	0,52	0,41	0,38	1,95	2,11	73,5	1,83
		DMFA	353	464	53,8	0,37	0,23	0,39	2,07	2,72	41,3	2,35
		ethanole+H2SO4	356	528	38,7	0,67	0,3	0,15	1,49	1,22	0,13	-
		vapor, INDO/S	318	398	50	0,8	0,73	0,18	1,93	1,15	10,1	-
30	1,4-di-5-(furyl-2)-1,3,4-oxa diazoly-2) benzole (FDPDF)	toluole	353	434	44,2	0,86	0,69	0,11	1,7	2,02	74,6	2,2
		ethanole	353	460	53,8	0,37	0,23	0,15	2,07	1,87	87,2	2,3
31	1,5-phenyl oxazolyl-2-4-[5-(thienyl-2)-1,3,4-oxa diazoly-2] benzole (POPDT)	toluole	335	422	47,62	0,66	0,57	0,3	1,83	1,53	35,6	2,6
		ethanole	336	422	42	0,78	0,5	0,11	1,62	1,60	31,9	2,9
32	2,5-di-(5-phenyl-oxazolyl-2) thiophen (POTOP)	toluole	390	468	48,2	0,36	0,40	0,70	1,85	1,30	2,9	4,8
		ethanol	386	458	42,4	0,40	0,42	0,63	1,63	1,46	3,0	4,53
		THF	389	457	41,5	0,48	0,49	5,53	1,6	1,25	3,1	4,45
		DMFA	390	436	43,9	0,33	0,35	0,70	1,69	1,59	2,8	4,22
		ethanole+H2SO4	405	512	44,7	0,72	0,32	0,13	1,72	1,51	1,0	-
		vapor, INDO/S	350	-	45,0	0,30	0,33	0,78	1,73	1,32	0,06	-
33	2-(5-phenyl oxazolil-2)-5-[5-phenyl-1,3,4-oxa diazoly-2] thiophen (POTDP)	toluole	373	452	43	0,39	0,43	0,68	1,62	1,82	6,1	4,8
		ethanole	379	452	43,1	0,45	0,47	0,57	1,66	1,28	2,7	4,43
		ethanole+H2SO4	401	522	41,3	0,72	0,32	0,12	1,59	2,5	0,13	-
		vapor, INDO/S	341	411	40	0,3	0,33	0,78	1,73	1,27	0,16	-
34	2-(5-phenyl-oxazolil-2)-5-[5-(thienyl-2)-1,3,4-oxa diazoly-2] thiophen (POTDT)	ethanole	378	460	49,6	0,38	0,42	0,68	1,91	1,42	4,34	5,2
		toluole	375	456	44,7	0,47	0,41	0,22	1,72	1,54	3,96	5,3

Notes. Solvents: 1,2,2'-TFTCE is 1,1,2,2'-trifluorotrichloroethanol; THF is tetrahydrofuran; DMFA is dimethylformamide; DMSO is dimethylsulfoxide; DiEG is diethyleneglycol; ethanole+H2SO4 is solution of H2SO4 in ethanol with pH $\approx$ 2,0; vapor, INDO/S is characteristics of the "free states" of the molecule by calculations by the LCAO-MO SCF extended-CI INDO/S methods; $\lambda_{\text{abs}}^{\text{max}}$, $\lambda_{\text{fl}}^{\text{max}}$ and $\lambda_{\text{gen}}^{\text{max}}$ are wavelength of the maxima in the absorption, FI and GRI spectra; $\epsilon_{\text{abs}}^{\text{max}}(\nu)$ is the molar's coefficient of extinction the absorption spectra; γ_{fl} is the QYFI, k_{fl} and k_{ST} is the RC FI and RC ItCC; $\sigma_{13}^{\text{abs}}(\nu)$ and $\sigma_{31}^{\text{osc}}(\nu)$ are the cross section for of the laser pump-pulse of the absorption spectra and for stimulated emission in the maxima of the wavelengths wide bands in the absorptions and fluorescence (298K) spectra; E_{lp} is the threshold density of energy absorbed of a single of the laser pump-pulse and average density of power, P_{lp} , at the frequency of following of pulses for $F_{\text{exit}} \approx 30$ Gz; t_{lp} is the limit of a single the laser pump-pulse at which occurrence the generated radiation of light is possible; vapor, laser are experimental characteristic molecules of vapors [1, 34 - 37].

For the compounds if values the cross sections $\sigma_{24}^*(\nu^{\text{osc}})$ and the cross sections $\sigma_{31}^{\text{osc}}(\nu)$ and $\sigma_{24}^*(\nu^{\text{osc}})$ but to the time t_{lp} up tends to about 100 ns are comparable, and GRI because $t_{\text{lp}} = 10^{-11} - 10^{-12}$ s is impossible in Fig. 4.

The increase in the steepness the limit front time of pump-pulse, t_{lp} should lower the lasing threshold, which should tend to the minimal possible of value.

Since the magnitude of losses related to the triplet-

triplet reabsorption spectra is increases in time, the limit of the dye-laser pulse is always shorter than the excitation of pumping ($\Delta\tau_{\text{osc}} < \Delta\tau_{\text{exit}}$) in Table 4.

The Spectrum Fluorescence and Losses at the Pump Electrons

The probability of emission $W_{\text{fl}}(E)$ is characterized by value of the ElQYFI (γ_{fl}^e), and also function of excitation which is proportional to total dependence on the energy of electrons and the sections of excitation $\sigma_i^{\text{exit}}(E)$ of all the STEIExSt according to

expression

$$W_{fl}(E) = (j/e)n_0 h\nu \sum_i \gamma_{fl}^e \sigma_i^{exit}(E), \quad (9)$$

where j is density of the current, e is charge of electrons, n_0 is concentration of molecules and $h\nu$ is the quant of light (or Fl). [4, 12]

Average on ensemble of compounds the values of the absorbed energy $\bar{E}_n$ and QYFl $\bar{\gamma}_{fl}$ will be defined ratio [12]

$$\bar{E}_n = \frac{\int \sigma_i^{exit}(E_{exit}) E_{exit} dE_{exit}}{\int \sigma_i^{exit}(E_{exit}) dE_{exit}} \quad (10)$$

and

$$\bar{\gamma}_{fl} = \frac{\int \sigma_i^{exit}(E_{exit}) \gamma_{fl}^e(E_{exit}) dE_{exit}}{\int \sigma_i^{exit}(E_{exit}) dE_{exit}} \quad (11)$$

Therefore the energy-QYFl (γ_{fl}^e) at the electron excited of compounds by formula [4]

$$\gamma_{fl}^e = \frac{\bar{E}_n \int \sigma_i^{exit}(E_{exit}) \gamma_{fl}^e(E_{exit}) dE_{exit}}{\int \sigma_i^{exit}(E_{exit}) E_{exit} dE_{exit}}, \quad (12)$$

where $\bar{E}_{fl}$ is average value of energy of the QYFl.

At the electric excitation of values EnQYFl it is appreciable less, than QYFl at optical excitation.

The Efficiency of Fluorescence Spectra and OLEDs

The power efficiency of the OLEDs-device with the standard diagram of the orientation of radiation is function of enclosed voltage U_{entr} and efficiency on the current γ_{cur} . The OLEDs-devices have the working voltage 5 - 8 - 14 V, and also can be reduced up to 3 - 4 V (29 lm/W) at brightness 500 - 1000 kd/m². For solid-state of OLEDs-diodes γ_{LED} ice makes 80 lm/W (at the current 20 mA sometimes up to 150 lm/W). [11]

The value γ_{LED} is calculated by formula

$$\gamma_{LED} = \gamma_{cur} (\pi/U_{entr}). \quad (13)$$

In view of what efficiency on the current (γ_{cur}) is defined by expression as

$$\gamma_{cur} = k\pi\gamma_{int}\gamma_{exit}, \quad \gamma_{LED} = \frac{\gamma_{LED}}{k\pi\gamma_{int}\gamma_{exit}} (1/U_{entr}), \quad (14)$$

where k is constant determined by function of photosensitivity of the human eye.

Best samples of the OLEDs-device have efficiency on current $\gamma_{cur} = (2 - 10)$ and sometimes 40 kd/A. [11]

The external quantum efficiencies γ_{int} , i.e. losses on

internal reflection in interfaces between the organic layers can achieve up to 80 %.

The external quantum efficiency (EQYFl) for OLEDs-diode γ_{exit} makes

$$\gamma_{exit} = 1 - \left[\sqrt{1 - (1/n_r^2)} \right], \quad (15)$$

where n_r is parameter of refraction of active layer OLEDs and at $n_r = 1,49$ value $\gamma_{exit} \leq 26$ %, at $n_r = 1,7$ value $\gamma_{exit} \leq 20$ %, and at $n_r = 2$ value the makes size $\gamma_{exit} \leq 13,4$ %. [4]

Reception of the intensives of luminescence with the given coordinates of chromaticity speaks the opportunity of thin selection STEExSt of materials in the OLEDs-device. [5,11]

In strong fields at intensity of the electric field between electrodes makes 10^6 - 10^7 A/cm² and process the electronic results to the auto-electronic emission issue and the amplification of electrons up to the energy, causing of the ElExEn and the photoionization. [11]

Thus, the power properties of any the optic-electronics device are defined by active the compounds or related the QYFl (γ_{fl}^i) and QYPh (γ_{ph}^i) by environments for which not only it is necessary to have the full set of the spectral-fluorescence characteristics, but also it is necessary to carry out authentic interpretations.

Conclusion

The spectral-luminescence by now spectral-calculations of technological methods is offered. The method which allows to establish the spectroscopic characteristics of compounds in the GrSt (S_0) and in the full spectra singlet and triplet STEExSt in different environments and also put into practice: 1) at different parameters of impulse-pumping to define required the spectral-power properties, and the energy-quantum efficiently, and also the energy of contribution for dye-lasers; 2) the fine structure of Raman scattering, and also of NMR-, IR- and UV-absorption, and Fl- and Ph-spectrums; 3) variations of the coefficient is the molyare extinctions, and of refraction or dispersion in vapor, solvent, and molecular crystals; 4) the absolute and relative of QYFl and the QYPh; 5) the parameters GRI in the dye-lasers; 6) the photo-stability and service life of dye.

REFERENCES

[1]A. E. Obukhov, Laser Physics, **7** (5), 1102 (1997).

- <http://www.lasphys.com/lasphys/submission-system>
- [2] *Spectroscopy of Ground and Excited States of the Multiatomic Molecules in Variation of Conditions*, edited by A. E. Obukhov, ("Sputnik+", Russia, Moscow, 2010). ББК 22.344. О-26. ISBN 978-5-9973-0657-1.
- [3] A. E. Obukhov, *Laser Physics*, **6**, 890 (1996).
- [4] A. E. Obukhov, *Proceedings of SPIE. Material Development for Organic Electronics and Photonics, 2012 Photonics Europe, Brussels, Belgium*, **8435**, 84351J-1 (2012).
- [5] A. E. Obukhov, *Sov. J. Quantum. Electronics*, **20**, 863 (1993).
- [6] Card file JCPDS "Joint Committee for Powder Diffraction Studies" - ICDD "International Centre for Diffraction Data" (1997).
- [7] D. H. Christensen, J. T. Nielsen and O. F. Nielsen, *J. of Molecular Spectroscopy*, **24**, Issue 1-4, 225 (1967). [http://dx.doi.org/10.1016/0022-2852\(67\)90084-7](http://dx.doi.org/10.1016/0022-2852(67)90084-7)
- [8] *Modern Spectroscopy*, edited by J. Michael Hollas. (Jon Wiley & Sons: West Sussex, England, 2004).
- [9] G. A. Abakumov, B. I. Polyakov, A. P. Simonov, et al., *Applied Physics B.*, **27 B**, Issue 1, 57 (1982). <http://link.springer.com/article/10.1007/BF00697297>.
- [10] P. P. Sorokin, J. R. Lancard, E. C. Hammond, and V. L. Moruzzi, *IBM J. Res. and Develop*, **11**, 130 (1967).
- [11] *Organic Electroluminescence*, edited by Kafafi Zakia

(Taylor & Francis Group. LLC. New-York, London, 2005).

- [12] A. Kazakov, A. Kukhta, and V. Suchkov, *J. of Fluorescence*, **10 (4)**, 409 (2000).



Alexandr Evgenievich Obukhov the date of birth is 29.10.1953 in Moscow. He graduated from Moscow Power Engineering Institute from 1970 to 1976, and he became a specialist in the field of mechanics engineering aviation devices. He graduated from Belorussian States

University from 1989 to 1992, and received a Ph.D. degree of the candidate of physical and mathematical sciences. In 1996 is lecturer of Physics in Moscow Mining State University, and also in 2010 senior scientist of Bauman Technical State University. Today A. E. Obukhov works as senior scientist in Moscow Power Engineering Institute "MPEI". In 2012 achieved degree doctor of the physical and mathematical science. A. E. Obukhov published more than 100 journal papers and one book "Spectroscopy of the Ground and Excited Electronic States of the Multiatomic Molecules in Variation of Conditions". His scientific interests: X-, E-, N-Ray and NMR-spectroscopy, Spatial and electronic structure of multiatomic compounds, Photophysics, Photochemistry and Photobiology, and the Nonlinear phenomena and the intermolecular quantum mechanisms of the multiphoton transitions in the full spectrum of the singlets and triplets electronic excited states on the dye-lasers, OLEDs, OTETs, IR-, SCR-, UV-absorptions, Raman scattering, Fluorescence and Phosphorescence, Emissions and Generation radiated of light, Photochemistry, Photobiology, Chemical reactions, Nanocurrent, and Nanotechnology, and other science.